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ANTIFERROMAGNETIC ORDERING AND PSEUDOGAP IN A MODEL OF QUASI-1D ORGANIC SUPERCONDUCTOR ELECTRONIC SUBSYSTEM

Yuriy Skorenkyy, Oleksandr Kramar
Ternopil Ivan Puluj National Technical University,
56 Ruska St, Ternopil, Ukraine; e-mail: skorenkyy@tstu.edu.ua

Nowadays, the diversity of synthesized organic compounds opens new prospects for industrial applications. Among those, organic compounds with electrical and magnetic properties similar to transition metal compounds attract much attention. Over a thousand molecular conductors and over a hundred molecular superconductors have been synthesized so far [1]. Typical molecular conductors possess non-integral oxidation states either through partial charge-transfer between a donor molecule and an acceptor molecule or through partial oxidation of a donor molecule which is a prerequisite for achieving partial filling of the conduction band. An alternative way of obtaining metallic conductance is to use a compound in which, though a number of electrons per lattice site is even, the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) is small [1]. Despite great efforts, the underlying mechanisms of peculiar features observed in strongly anisotropic molecular superconductors remain unclear. We have carried out a theoretical investigation of electronic subsystem of Fabre salts $(TMTTF)_2X$ (here TMTTF denotes tetrametyl-tetrathiafulvalene molecule, X stands for monovalent anion PF_6,AsF_6, ClO_4 or Br) and Bechgaard salts $(TMTSF)_2X$ (here TMTSF stands for tetrametyl-tetraselenfulvalene which differs from TMTTF by substitution of S by Se) with special attention to microscopical mechanism for antiferromagnetic order stabilization and pseudogap formation in the electronic spectrum. In these systems the overlap of wavefunctions of sites belonging to one chain is much larger than the interchain overlap, resulting in one-dimensional conductance in which electronic correlations play an essential role [2]. For consistent description of electron correlations, including the correlated hopping of electrons, we use the configurational representation of the microscopical model [3] taking into account translation processes with nearest-neighbors and next-nearest-neighbors hopping parameters between TMTSF (TMTTF) sites dependent on the applied external pressure or doping of anion subsystem as well as intra- and intersite Coulomb interactions and intersite exchange interaction. Study of the quasi-particle spectrum calculated within the Green function method proves that the strong electron correlations lead to realization of the conductor-to-insulator and paramagnet-antiferromagnet phase transitions. In the insulator state, energy gap opens in the energy spectrum on Fermi surface or part of it. For the latter case, we obtained the energy gap dependance on the wave vector and interpreted its peculiarities. Conditions for pseudogap opening in the spectrum and anomalies in dispersion of current carriers (known as hot spots) are determined. Next-nearest-neighbor hopping is shown to break the perfect nesting property and destabilize antiferromagnetic state. On the basis of these results, experimental phase diagrams for quasi-onedimensional organic superconductors $(TMTSF)_2X$ and $(TMTTF)_2X$ are interpreted.

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